

CLAIMS

What is claimed as new and desired to be protected by Letters Patent of the United States is:

1. A system for improved simulation of a biological system comprising a plurality of
5 chemical reactions, the system comprising:

a modeling component for constructing a model of a biological system including a first chemical reaction and a second chemical reaction; and

a simulation engine accepting as input said constructed model of the biological system and generating as output dynamic behavior of the biological system using a first type of
10 computational model for the first chemical reaction and a second type of computational model for the second chemical reaction.

2. The system of claim 1 wherein the modeling component allows construction of a block diagram model of the biological system.

3. The system of claim 2 wherein the modeling component further includes at least
15 one block identifying a set of related chemical reactions.

4. The system of claim 1 wherein the modeling component includes a graphical user interface for accepting user commands and data.

5. The system of claim 1 wherein said first type of computational model is selected from the group consisting of ordinary differential equation analysis, partial differential
20 equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

6. The system of claim 5 wherein said second type of computational model is selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and
25 stochastic analysis.

7. The system of claim 1 wherein said second type of computational model is selected from the group consisting of ordinary differential equation analysis, partial

differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

8. The system of claim 1 further comprising an analysis environment in communication with said simulation engine, said analysis environment displaying the
5 dynamic behavior of the biological system.

9. An improved method for simulation of a biological system including a first chemical reaction and a second chemical reaction, the method comprising the steps of:

(a) constructing a model of the biological system including a first chemical reaction and a second chemical reaction; and

10 (b) generating dynamic behavior of the modeled biological system using a first type of computational model for the first chemical reaction and a second type of computational model for the second chemical reaction.

10. The method of claim 9 wherein step (a) comprises constructing a block diagram model of the biological system.

15 11. The method of claim 10 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

12. The method of claim 9 wherein step (a) comprises:

(i) providing a graphical user interface for accepting user commands and data;
and

20 (ii) constructing a model of the biological system including a first chemical reaction and a second chemical reaction using the user commands and data.

13. The method of claim 9 wherein step (b) comprises:

(i) generating an expected result of the first chemical reaction using a computational model selected from the group consisting of ordinary differential equation analysis, partial
25 differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis; and

(ii) generating an expected result of the second chemical reaction.

14. The method of claim 9 wherein step (b) comprises:

(i) generating an expected result of the first chemical reaction; and

(ii) generating an expected result of the second chemical reaction using a

5 computational model selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

15. The method of claim 9 further comprising the step of displaying the expected result.

10 16. An article of manufacture having embodied thereon computer-readable program means for improved simulation of a biological system comprising a plurality of chemical reactions, the article of manufacture comprising:

computer-readable program means for constructing, using the received user commands and data, a model of a biological system including a first chemical reaction and a
15 second chemical reaction;

computer-readable program means for generating, using the constructed model of the biological system, dynamic behavior of the modeled biological system using a first type of computational model for the first chemical reaction and a second type of computational model for the second chemical reaction.

20 17. The article of manufacture of claim 16 further comprising computer-readable program means for displaying the dynamic behavior that is generated.

18. The article of manufacture of claim 16 wherein said computer-readable program means for constructing a model of the biological system comprises computer-readable program means for constructing a block diagram model of the biological system.

25 19. The article of manufacture of claim 16 wherein said computer-readable program means for constructing a block diagram model of the biological system includes computer-

readable program means for constructing at least one block identifying a set of related chemical reactions.

20. The article of manufacture of claim 16 wherein computer-readable program means for generating dynamic behavior of the modeled biological system comprises
5 computer-readable program means for generating an expected result of the first chemical reaction using a computational model selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

21. The article of manufacture of claim 16 wherein computer-readable program
10 means for generating dynamic behavior of the modeled biological system comprises computer-readable program means for generating an expected result of the second chemical reaction using a computational model selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

15 22. The article of manufacture of claim 16 further comprises computer-readable program means for displaying the expected results.

23. A system for improved simulation of chemical reactions comprising:

a modeling component for constructing a model of a first chemical reaction and a second chemical reaction; and

20 a simulation engine accepting as input said constructed model of the chemical reaction and generating as output an expected result using a first type of computational model for the first chemical reaction and a second type of computational model for the second chemical reaction.

24. The system of claim 23 wherein the modeling component allows construction of
25 a block diagram model of the first chemical reaction and the second chemical reaction.

25. The system of claim 24 wherein the modeling component further includes at least one block identifying a set of related chemical reactions.

26. The system of claim 23 wherein the modeling component includes a graphical user interface for accepting uses commands and data.

27. The system of claim 23 wherein said first type of computational model is selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

28. The system of claim 27 wherein said second type of computational model is selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

29. The system of claim 23 wherein said second type of computational model is selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

30. The system of claim 23 further comprising an analysis environment in communication with said simulation engine, said analysis environment displaying the expected result.

31. An improved method for simulation of chemical reactions, the method comprising the steps of:

(a) constructing a model of a first chemical reaction and a second chemical reaction; and

(b) generating an expected result of the first modeled chemical reaction using a first type of computational model and generating a second modeled chemical reaction for the second chemical reaction using a second type of computational model.

32. The method of claim 31 wherein step (a) comprises constructing a block diagram model of the first chemical reaction and the second chemical reaction.

33. The method of claim 32 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

34. The method of claim 31 wherein step (a) comprises:

(i) providing a graphical user interface for accepting user commands and data;

5 and

(ii) constructing a model of a first chemical reaction and a second chemical reaction using the user commands and data.

35. The method of claim 31 wherein step (b) comprises:

10 (i) generating an expected result of the first chemical reaction using a computational model selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis; and

(ii) generating an expected result of the second chemical reaction.

36. The method of claim 31 wherein step (b) comprises:

15 (i) generating an expected result of the first chemical reaction; and

(ii) generating an expected result of the second chemical reaction using a computational model selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

20 37. The method of claim 31 further comprising the step of displaying the expected result.

38. An article of manufacture having embodied thereon computer-readable program means for improved simulation of chemical reactions, the article of manufacture comprising:

25 computer-readable program means for constructing a model of a first chemical reaction and a second chemical reaction;

computer-readable program means for generating an expected result for the first chemical reaction using a first type of computational model and generating an expected result for the second chemical reaction using a second type of computational model.

39. The article of manufacture of claim 38 further comprising computer-readable
5 program means for displaying the expected result.

40. The article of manufacture of claim 38 wherein said computer-readable program means for constructing a model of the chemical reactions comprises computer-readable program means for constructing a block diagram model of a chemical reaction.

41. The article of manufacture of claim 38 wherein said computer-readable program
10 means for constructing a block diagram model of the chemical reaction includes computer-readable program means for constructing at least one block identifying a set of related chemical reactions.

42. The article of manufacture of claim 38 wherein computer-readable program means for generating an expected result of the modeled chemical reaction comprises
15 computer-readable program means for generating an expected result of the first chemical reaction using a computational model selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

43. The article of manufacture of claim 38 wherein computer-readable program
20 means for generating an expected result of the modeled chemical reaction comprises computer-readable program means for generating an expected result of the second chemical reaction using a computational model selected from the group consisting of ordinary differential equation analysis, partial differential equation analysis, difference equation analysis, algebraic equation analysis, and stochastic analysis.

25 44. The article of manufacture of claim 38 further comprises computer-readable program means for displaying the expected result.